Marc Kac Seminar

Metastable dynamics of Allen–Cahn equations

Nils Berglund

MAPMO, Université d'Orléans

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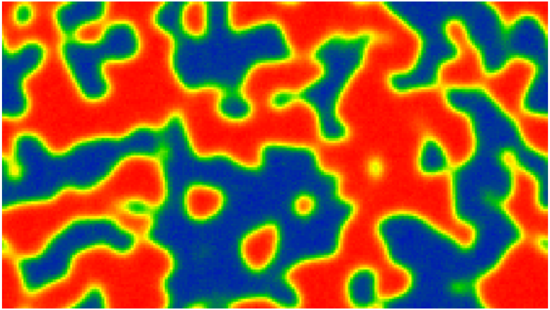
Joint works with Giacomo Di Gesù (Vienna), Bastien Fernandez (Paris),
Barbara Gentz (Bielefeld) and Hendrik Weber (Warwick)

Part I. Models and results



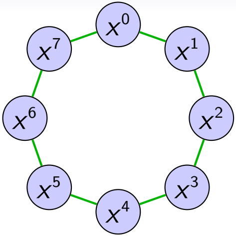
Metastability

A metastable system: supercooled water

(Source: https://youtu.be/fSPzMva9_CE)

Examples of particle systems

Example 1 [B, Fernandez, Gentz, Nonlinearity 2007]



- N particles on a circle $\mathbb{Z}/N\mathbb{Z}$
- Bistable local dynamics
- Ferromagnetic nearest neighbour coupling
- Independent noise on each site

$$\mathrm{d}x_t^i = \left[x_t^i - (x_t^i)^3\right]\mathrm{d}t + \frac{\gamma}{2}\left[x_t^{i+1} - 2x_t^i + x_t^{i-1}\right]\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t^i$$

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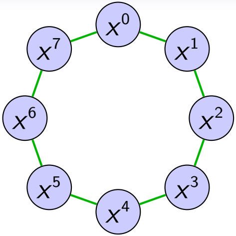

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Gradient system $\quad \mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$

potential $V(x) = \sum_i U(x^i) + \frac{\gamma}{4}\sum_i (x^{i+1} - x^i)^2 \qquad U(\xi) = \frac{1}{4}\xi^4 - \frac{1}{2}\xi^2$

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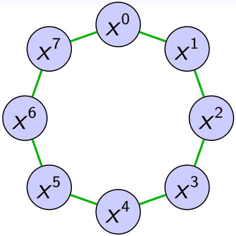

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Example 2 Replace circle by 2D torus $(\mathbb{Z}/N\mathbb{Z})^2$

Example 3 [B, Dutercq, J Stat Phys 2016]: Same V + constraint $\sum_i x^i = 0$

General gradient systems with noise

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

$V : \mathbb{R}^N \to \mathbb{R}$: confining potential, class $\mathcal{C}^2$

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- ▷ Stationary points: $\mathcal{X} = \{x : \nabla V(x) = 0\}$
- ▷ Local minima: $\mathcal{X}_0 = \{x \in \mathcal{X} :$ all ev of Hessian $\nabla^2 V(x)$ are $> 0\}$
- ▷ Saddles of index 1: $\mathcal{X}_1 = \{x \in \mathcal{X} : \nabla^2 V(x)$ has 1 negative ev $\}$

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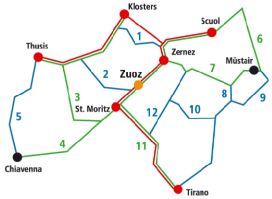
Dynamics ~ markovian jump process on $\mathcal{G} = (\mathcal{X}_0, \mathcal{E})$, $\mathcal{E} \subset \mathcal{X}_1$



Rot Rhätische Bahn
Grün ganzjährig offen
Blau Wintersperre

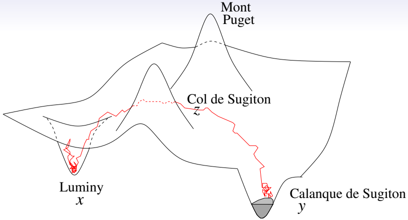
Nr.	Pass	Land	Passhöhe (m.ü.M.)
1	Flüela	CH	2383
2	Albula	CH	2312
3	Julier	CH	2284
4	Maloja	CH	1815
5	Splügen	I - CH	2115
6	Reschen	A - I	1507
7	Ofen	CH	2149
8	Umbrail	CH - I	2502
9	Stilfserjoch	I	2757
10	Foscagno	I	2291
11	Bernina	CH - I	2323
12	Fla. di Livigno	I	2315

The double-well case

$$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

$V : \mathbb{R}^d \to \mathbb{R}$ confining potential

$\tau_y^x = \inf\{t > 0 \colon x_t \in \mathcal{B}_\varepsilon(y)\}$
first-hitting time of small ball $\mathcal{B}_\varepsilon(y)$, when starting in x



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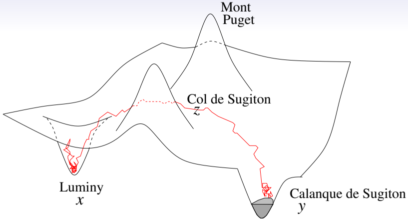

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Arrhenius' law (1889): $\mathbb{E}[\tau_y^x] \simeq e^{[V(z)-V(x)]/\varepsilon}$

Eyring–Kramers law (1935, 1940):
Eigenvalues of Hessian of V at minimum x: $0 < \nu_1 \leqslant \nu_2 \leqslant \dots \leqslant \nu_d$
Eigenvalues of Hessian of V at saddle z: $\lambda_1 < 0 < \lambda_2 \leqslant \dots \leqslant \lambda_d$

$$\mathbb{E}[\tau_y^x] = 2\pi\sqrt{\frac{\lambda_2 \dots \lambda_d}{|\lambda_1|\nu_1 \dots \nu_d}}\, e^{[V(z)-V(x)]/\varepsilon}\left[1 + \mathcal{O}_\varepsilon(1)\right]$$

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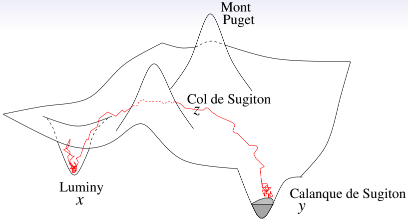

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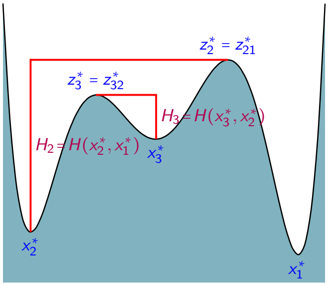
Arrhenius' law: proved by Freidlin, Wentzell (1979) using large deviations

Eyring–Kramers law: Bovier, Eckhoff, Gayrard, Klein (2004) using potential theory, Helffer, Klein, Nier (2004) using Witten Laplacian, . . .

More than two wells

Definition: Communication height

$$H(x_i^*, x_j^*) = \inf_{\gamma: x_i^* \to x_j^*} \sup_t V(\gamma_t) - V(x_i^*)$$
$$= V(z_{ij}^*) - V(x_i^*)$$



Definition: Metastable hierarchy

$x_1^* \prec x_2^* \prec \dots \prec x_n^* \Leftrightarrow \exists \theta > 0\colon \ \forall k$

$$H_k := H(x_k^*, \{x_1^*, \dots, x_{k-1}^*\})$$
$$\leqslant \min_{i<k} H(x_i^*, \{x_1^*, \dots, x_{i-1}^*, x_{i+1}^*, \dots, x_k^*\}) - \theta$$

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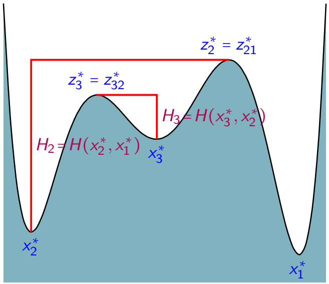

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Theorem: Eyring–Kramers law [Bovier,Eckhoff,Gayrard,Klein 2004]

τ_k = first-hitting time of nbh of $\{x_1^*, \dots, x_k^*\}$ $\qquad \lambda_k = k^{\text{th}}$ ev of generator

$$\mathbb{E}^{x_k^*}[\tau_{k-1}] = \frac{2\pi}{|\lambda_-(z_k^*)|}\sqrt{\frac{|\det \nabla^2 V(z_k^*)|}{\det \nabla^2 V(x_k^*)}}\, e^{H_k/\varepsilon}\big[1 + \mathcal{O}_\varepsilon(1)\big] \simeq |\lambda_k|^{-1}$$

Potential landscape for Example 1

$$V(x) = \sum_{i\in\mathbb{Z}/N\mathbb{Z}} U(x^i) + \frac{\gamma}{4}\sum_{i\in\mathbb{Z}/N\mathbb{Z}} (x^{i+1}-x^i)^2 \qquad U(\xi) = \tfrac{1}{4}\xi^4 - \tfrac{1}{2}\xi^2$$

$\gamma = 0$: $\mathcal{X} = \{-1,0,1\}^N$, $\mathcal{X}_0 = \{-1,1\}^N$, $\mathcal{X}_1 = \{x \in \mathcal{X} \colon \text{one } x^i = 0\}$

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Theorem [BFG, Nonlinearity 2007]

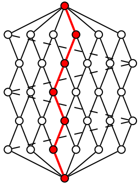
No bifurcation for $0 \leqslant \gamma \leqslant \gamma^*(N)$

where $\gamma^*(N) > \frac{1}{4} \quad \forall N \geqslant 2$

$V_\gamma(z^*_\gamma) = V_0(z^*_0) + \gamma(\#\text{ interfaces}) + \cdots$

Ising-like dynamics

+	+	+	+	+	+
−	+	+	+	+	+
−	+	+	+	+	−
−	+	+	+	−	−
−	−	+	+	−	−
−	−	+	−	−	−
−	−	−	−	−	−



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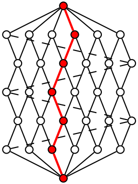

Theorem [BFG, Nonlinearity 2007]

$\gamma > \dfrac{1}{2\sin^2(\pi/N)} \Leftrightarrow \mathcal{X}_0 = \{\pm(1,\dots,1)\}, \ \mathcal{X}_1 = \{0\} \Leftrightarrow$ Synchronization

Transition to synchronization

Symmetry group

$G = D_N \times \mathbb{Z}_2 = \langle r, s, c \rangle$

$$r(x) = (x^2, x^3, \dots, x^N, x^1)$$
$$s(x) = (x^N, x^{N-1}, \dots, x^1)$$
$$c(x) = -x$$

$\mathcal{X}$ partitionned into
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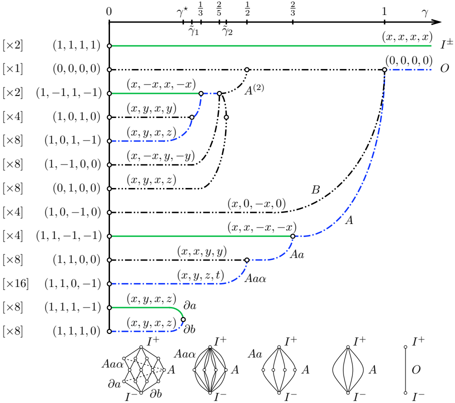
Useful to study bifurcation diagram



Example: $N = 4$, $|\mathcal{X}| = 3^4$ for $\gamma = 0$

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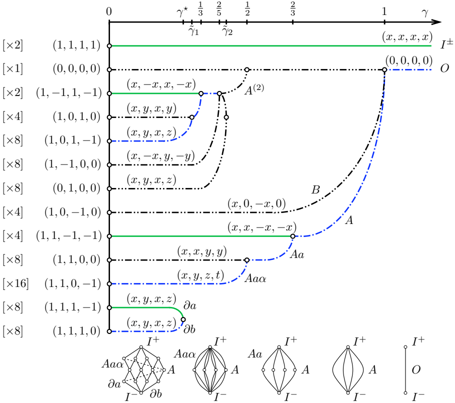

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Problem: no metastable hierarchy ⇒ Usual Eyring–Kramers law invalid

Limitations of the standard Eyring–Kramers law

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  What happens when V is invariant under a group of symmetries?
  (no metastable hierarchy)

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  What happens when $\gamma \sim N^2$ and $N \to \infty$ in example 1?
  One expects convergence to Allen–Cahn SPDE

$$\partial_t u(t,x) = \frac{\gamma}{N^2} \Delta u(t,x) + u(t,x) - u(t,x)^3 + \sqrt{2\varepsilon}\xi(t,x)$$

  where ξ is space-time white noise

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Limitations of the standard Eyring–Kramers law

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  Representation theory of finite groups → clustering of eigenvalues [B, Dutercq, JoTP 2015]

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Deterministic Allen–Cahn PDE

[Chafee & Infante 74, Allen & Cahn 75]

$$\partial_t u(x,t) = \partial_{xx} u(x,t) + f(u(x,t))$$

- $x \in [0, L]$, L: bifurcation parameter
- $u(x,t) \in \mathbb{R}$
- Either periodic or zero-flux Neumann boundary conditions
- In this talk: $f(u) = u - u^3$ (results more general)

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Energy function:

$$V[u] = \int_0^L \Big[\frac{1}{2}u'(x)^2 - \frac{1}{2}u(x)^2 + \frac{1}{4}u(x)^4\Big]\,\mathrm{d}x \qquad \to \quad \text{min}$$

Scaling limit of particle system of Example 1 with $\gamma = 2\frac{N^2}{L^2}$

Stationary solutions: $u_0''(x) = -u_0(x) + u_0(x)^3$ critical points of V

Stationary solutions

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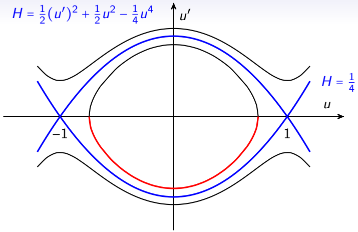
- $u_\pm(x) \equiv \pm 1$
- $u_0(x) \equiv 0$
- Nonconstant solutions satisfying b.c.
  (expressible in terms of Jacobi elliptic fcts)



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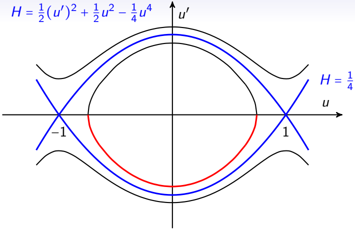

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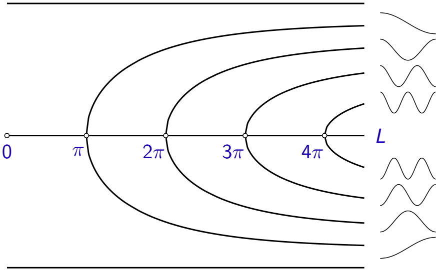
- ▷ Neumann b.c: $2k$ nonconstant solutions when $L > k\pi$



- ▷ Periodic b.c: k families when $L > 2k\pi$

Stability of stationary solutions

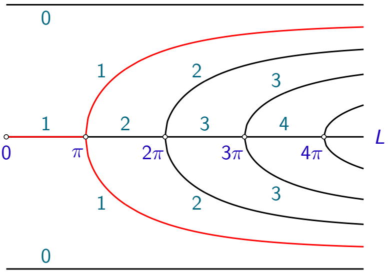
$u_0''(x) = -u_0(x) + u_0(x)^3$

Variational eq around u_0: $\partial_t v_t(x) = v_t''(x) + [1 - 3u_0(x)^2]v_t(x)$

Sturm–Liouville spectrum of RHS determines stability of u_0

- $u_\pm \equiv \pm 1$: always stable (global minima of V)
- $u_0 \equiv 0$: always unstable, eigenvalues $-\lambda_k = 1 - \left(\frac{\beta k \pi}{L}\right)^2$
  (Neumann b.c.: $\beta = 1$, periodic b.c.: $\beta = 2$)

Neumann b.c.:
Number of positive eigenvalues
(= unstable directions)
Transition state



Coarsening dynamics

[Carr & Pego 89, Chen 04] (Link to simulation)

Coarsening dynamics with noise

(Link to simulation)

Eyring–Kramers law for 1D SPDEs: heuristics

$$\dot{u}_t(x) = \Delta u_t(x) + f(u_t(x)) \quad + \sqrt{2\varepsilon}\,\xi(t,x) \qquad (\Delta \equiv \partial_{xx}, f(u) = u - u^3)$$

Initial condition: u_{in} near $u_- \equiv -1$ with eigenvalues ν_k

Target: $u_+ \equiv 1$, $\tau_+ = \inf\{t > 0 \colon \|u_t - u_+\|_{L^\infty} < \rho\}$

Transition state: ($\beta = 1$ for Neumann b.c., $\beta = 2$ for periodic b.c.)

$$u_{\text{ts}}(x) = \begin{cases} u_0(x) \equiv 0 & \text{if } L \leqslant \beta\pi \quad \text{with ev } \lambda_k = (\frac{\beta k \pi}{L})^2 - 1 \\ u_1(x) \ \beta\text{-kink stationary sol.} & \text{if } L > \beta\pi \quad \text{with ev } \lambda'_k \end{cases}$$

Eyring–Kramers law for 1D SPDEs: heuristics

$$\dot{u}_t(x) = \Delta u_t(x) + f(u_t(x)) \;\; + \sqrt{2\varepsilon}\,\xi(t,x) \qquad (\Delta \equiv \partial_{xx}, f(u) = u - u^3)$$

Initial condition: u_{in} near $u_- \equiv -1$ with eigenvalues ν_k

Target: $u_+ \equiv 1$, $\tau_+ = \inf\{t > 0 \colon \|u_t - u_+\|_{L^\infty} < \rho\}$

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[Faris & Jona-Lasinio 82]: large-deviation principle

$\Rightarrow$ Arrhenius law: $\mathbb{E}^{u_{\text{in}}}[\tau_+] \simeq e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon}$

[Maier & Stein 01]: formal computation; for Neumann b.c.

$\Rightarrow \mathbb{E}^{u_{\text{in}}}[\tau_+] \simeq 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}}\, e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon}$

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- Rigorous proof?
- What happens when $L \to \beta\pi$ as then $\lambda_1 \to 0$?

Eyring–Kramers law for 1D SPDEs: main result

Theorem: Neumann b.c. [B & Gentz, Elec J Proba 2013]

- If $L < \pi - c$ with $c > 0$, then

$$\mathbb{E}^{u_{\rm in}}[\tau_+] = 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}} \, e^{(V[u_{\rm ts}]-V[u_-])/\varepsilon} \big[1 + \mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|^{3/2})\big]$$

- If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles) and λ'_k instead of λ_k

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- If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles) and λ'_k instead of λ_k
- If $\pi - c \leqslant L \leqslant \pi$, then

$$\mathbb{E}^{u_{\rm in}}[\tau_+] = 2\pi \sqrt{\frac{\lambda_1 + \sqrt{3\varepsilon/2L}}{|\lambda_0|\nu_0\nu_1} \prod_{k=2}^{\infty} \frac{\lambda_k}{\nu_k}}\, \frac{\mathrm{e}^{(V[u_{\rm ts}]-V[u_-])/\varepsilon}}{\Psi_+(\lambda_1/\sqrt{3\varepsilon/2L})} \bigl[1 + R(\varepsilon)\bigr]$$

  where Ψ_+ explicit, involves Bessel function $K_{1/4}$, $\lim_{\alpha\to\infty} \Psi_+(\alpha) = 1$
- If $\pi \leqslant L \leqslant \pi + c$, then same formula, with another function Ψ_-, involving Bessel functions $I_{\pm 1/4}$, $\lim_{\alpha\to\infty} \Psi_-(\alpha) = 2$

Eyring–Kramers law for 1D SPDEs: comments

- ▷ Periodic b.c.: similar result [B & Gentz, Elec J Proba 2013]
  For $L > 2\pi$: extra factor $\sqrt{\varepsilon}$ because saddle is a whole curve
- ▷ Proof: relies on spectral Galerkin approximation
- ▷ Similar results by F. Barret [Annales IHP, 2015]
  using different method (no bifurcation points, f more general)

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  using different method (no bifurcation points, f more general)

- For Neumann b.c. and $L < \pi$: ratio of spectral or Fredholm determinants in prefactor is explicitly computable (Euler product formulas)

$$\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k} = \frac{1}{2} \prod_{k=1}^{\infty} \frac{\left(\frac{k\pi}{L}\right)^2 - 1}{\left(\frac{k\pi}{L}\right)^2 + 2} = \frac{1}{2} \prod_{k=1}^{\infty} \frac{1 - \left(\frac{L}{k\pi}\right)^2}{1 + 2\left(\frac{L}{k\pi}\right)^2} = \frac{\sin(L)}{\sqrt{2}\sinh(\sqrt{2}L)}$$

  Similar expression for periodic b.c. and $L < 2\pi$

- For larger L, techniques for Feynman path integrals allow to compute the spectral determinants in prefactors [Maier & Stein]

The two-dimensional case

(Link to simulation)

The two-dimensional case

- ▷ Large-deviation principle: [Hairer & Weber, Ann. Fac. Sc. Toulouse, 2015]
- ▷ Naive computation of prefactor fails:

$$\log \prod_{k \in (\mathbb{N}^2)^*} \frac{1 - \left(\frac{L}{|k|\pi}\right)^2}{1 + 2\left(\frac{L}{|k|\pi}\right)^2} \simeq \sum_{k \in (\mathbb{N}^2)^*} \log\left(1 - \frac{3L^2}{|k|^2\pi^2}\right)$$

$$\simeq - \sum_{k \in (\mathbb{N}^2)^*} \frac{3L^2}{|k|^2\pi^2} \simeq -\frac{3L^2}{\pi^2} \int_1^\infty \frac{r\,\mathrm{d}r}{r^2} = -\infty$$

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- In fact, the equation needs to be renormalised

Theorem: [Da Prato & Debussche 2003]

Let ξ^δ be a mollification on scale δ of white noise. Then

$$\partial_t u = \Delta u + \left[1 + 3\varepsilon C(\delta)\right] u - u^3 + \sqrt{2\varepsilon}\xi^\delta$$

with $C(\delta) \simeq \log(\delta^{-1})$ admits local solution converging as $\delta \to 0$
(Global version: [Mourrat & Weber 2015])
[Mourrat & Weber 2014]: Renormalised eq = scaling limit of Ising–Kac model

Main result in dimension 2

Theorem: [B, Di Gesù, Weber 2016]

For appropriate $A \ni u_-$, $B \ni u_+$, $\exists \mu_N$ probability measures on ∂A:

$$\limsup_{N\to\infty} \mathbb{E}^{\mu_N}\big[\tau_B\big] \leqslant \frac{2\pi}{|\lambda_0|}\sqrt{\prod_{k\in\mathbb{Z}^2} \frac{|\lambda_k|}{\nu_k}\,e^{\frac{\nu_k-\lambda_k}{|\lambda_k|}}}\, e^{(V[u_{\rm ts}]-V[u_-])/\varepsilon}\big[1+c_+\sqrt{\varepsilon}\,\big]$$

$$\liminf_{N\to\infty} \mathbb{E}^{\mu_N}\big[\tau_B\big] \geqslant \frac{2\pi}{|\lambda_0|}\sqrt{\prod_{k\in\mathbb{Z}^2} \frac{|\lambda_k|}{\nu_k}\,e^{\frac{\nu_k-\lambda_k}{|\lambda_k|}}}\, e^{(V[u_{\rm ts}]-V[u_-])/\varepsilon}\big[1-c_-\varepsilon\big]$$

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(Inverse of) prefactor involves Carleman–Fredholm determinant:

$$\det{}_2(\mathrm{Id}+T) = \det(\mathrm{Id}+T)\mathrm{e}^{-\operatorname{Tr} T}$$

Defined whenever T is Hilbert–Schmidt, but not necessarily trace class

Applied here to $T = [(-\Delta+2)-(-\Delta-1)](|-\Delta-1|)^{-1} = 3(|-\Delta-1|)^{-1}$

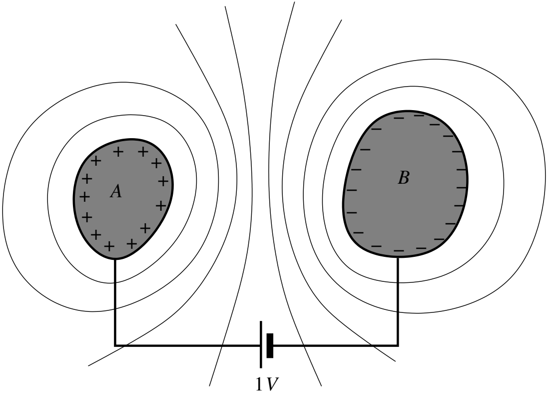
Outlook

- Dim $d = 3$: more difficult because 2 renormalisation constants needed
- More than two wells: understood in $d = 1$ (with symmetries in $\mathbb{R}^n$)

References: Particle system: [1]; nonquadratic: [2,3]; SPDEs: [4,5]; symmetries: [6,7];

1. N. B., Bastien Fernandez and Barbara Gentz, *Metastability in interacting nonlinear stochastic differential equations I: From weak coupling to synchronisation* & *II: Large-N behaviour*, Nonlinearity **20**, 2551–2581; 2583–2614 (2007)
2. N. B. and Barbara Gentz, *Anomalous behavior of the Kramers rate at bifurcations in classical field theories*, J. Phys. A: Math. Theor. **42**, 052001 (2009)
3. ______, *The Eyring–Kramers law for potentials with nonquadratic saddles*, Markov Processes Relat. Fields **16**, 549–598 (2010)
4. ______, *Sharp estimates for metastable lifetimes in parabolic SPDEs: Kramers' law and beyond*, Electronic J. Probability **18**, (24):1–58 (2013)
5. N. B., Giacomo Di Gesù, Hendrik Weber, *An Eyring–Kramers law for the stochastic Allen–Cahn equation in dimension two*, preprint (2016), `arXiv/1604.05742`
6. N. B. and Sébastien Dutercq, *The Eyring–Kramers law for Markovian jump processes with symmetries*, J. Theoretical Probability, First Online (2015)
7. ______, *Interface dynamics of a metastable mass-conserving spatially extended diffusion*, J. Statist. Phys. **162**, 334–370 (2016)

Part II. Proofs

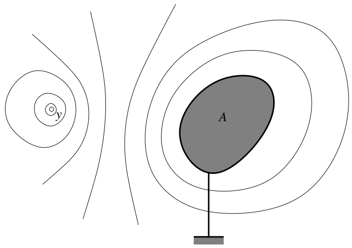


Potential theory and Eyring–Kramers law

Consider first Brownian motion $W_t^x = x + W_t$

Fact 1: $w_A(x) = \mathbb{E}[\tau_A^x]$ satisfies

$$\begin{cases} -\frac{1}{2}\Delta w_A(x) = 1 & x \in A^c \\ w_A(x) = 0 & x \in A \end{cases}$$



Green's function:

$-\frac{1}{2}\Delta G_{A^c}(x,y) = \delta(x-y)$

$\Rightarrow w_A(x) = \int_{A^c} G_{A^c}(x,y)\,\mathrm{d}y$

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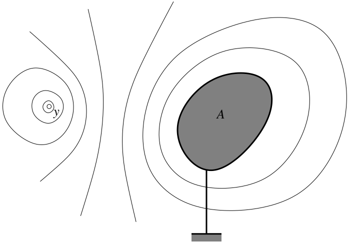

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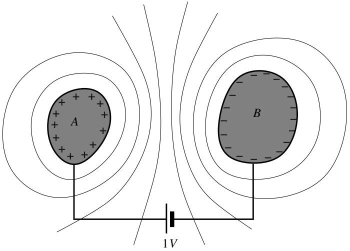
Fact 2: $h_{A,B}(x) = \mathbb{P}[\tau_A^x < \tau_B^x]$ satisfies

$$\begin{cases} -\frac{1}{2}\Delta h_{A,B}(x) = 0 & x \in (A \cup B)^c \\ h_{A,B}(x) = 1 & x \in A \\ h_{A,B}(x) = 0 & x \in B \end{cases}$$



$\rho_{A,B}$: "surface charge density" on ∂A

$$\Rightarrow h_{A,B}(x) = \int_{\partial A} G_{B^c}(x,y)\,\rho_{A,B}(\mathrm{d}y)$$

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Capacity: $\mathrm{cap}_A(B) = \int_{\partial A} \rho_{A,B}(\mathrm{d}y) \;\Rightarrow\; \nu_{A,B}(\mathrm{d}y) = \frac{\rho_{A,B}(\mathrm{d}y)}{\mathrm{cap}_A(B)}$ prob measure

Variational representation: Dirichlet form

$$\mathrm{cap}_A(B) = \int_{(A\cup B)^c} \|\nabla h_{A,B}(x)\|^2 \,\mathrm{d}x = \inf_{h\in\mathcal{H}_{A,B}} \int_{(A\cup B)^c} \|\nabla h(x)\|^2 \,\mathrm{d}x$$

($\mathcal{H}_{A,B}$: set of sufficiently smooth functions satisfying b.c.)

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Key observation: let $C = \mathcal{B}_\varepsilon(x)$, then (using $G(y,z) = G(z,y)$)

$$\begin{aligned}\int_{A^c} h_{C,A}(y)\,\mathrm{d}y &= \int_{A^c}\int_{\partial C} G_{A^c}(y,z)\rho_{C,A}(\mathrm{d}z)\,\mathrm{d}y \\ &= \int_{\partial C} w_A(z)\rho_{C,A}(\mathrm{d}z) = \text{cap}_C(A)\mathbb{E}^{\nu_{C,A}}[w_A]\end{aligned}$$

Harnack inequalities $\Rightarrow$ $\mathbb{E}^x[\tau_A] \simeq \mathbb{E}^{\nu_{C,A}}[w_A] = \dfrac{1}{\text{cap}_C(A)} \displaystyle\int_{A^c} h_{C,A}(y)\,\mathrm{d}y$

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General case: replace $\frac{1}{2}\Delta$ by $\varepsilon\Delta - \nabla V(x)\cdot\nabla$ and $\mathrm{d}x$ by $\mathrm{e}^{-V(x)/\varepsilon}\,\mathrm{d}x$

Potential-theoretic proof

"Magic" formula: for $A, B \subset \mathbb{R}^d$ disjoint sets,

$$\mathbb{E}^{\nu_{A,B}}[\tau_B] = \frac{1}{\mathrm{cap}_A(B)} \int_{B^c} h_{A,B}(y)\, \mathrm{e}^{-V(y)/\varepsilon}\, \mathrm{d}y$$

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Proving Eyring–Kramers formula: x starting well, y target well, z saddle
A and B small sets around x and y

- ▷ Variational arguments: $\operatorname{cap}_A(B) \simeq \varepsilon \sqrt{\frac{|\lambda_1|}{2\pi\varepsilon}} \sqrt{\frac{(2\pi\varepsilon)^{d-1}}{\lambda_2 \dots \lambda_d}}\, \mathrm{e}^{-V(z)/\varepsilon}$
- ▷ Laplace asymptotics: $\int_{B^c} h_{A,B}(y)\, \mathrm{e}^{-V(y)/\varepsilon}\, \mathrm{d}y \simeq \sqrt{\frac{(2\pi\varepsilon)^d}{\nu_1 \dots \nu_d}}\, \mathrm{e}^{-V(x)/\varepsilon}$
- ▷ Use Harnack inequalities to show that $\mathbb{E}^{\nu_{A,B}}[\tau_B] \simeq \mathbb{E}^{x}[\tau_B]$
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Eyring–Kramers formula:

$$\mathbb{E}^x[\tau_B] = 2\pi \sqrt{\frac{\lambda_2 \dots \lambda_d}{|\lambda_1| \nu_1 \dots \nu_d}} \, e^{[V(z)-V(x)]/\varepsilon} \left[1 + \mathcal{O}_\varepsilon(1)\right]$$

Eyring–Kramers law for nonquadratic saddles

Theorem: [B & Gentz, MPRF 2010]

- Saddle in 0, separating A and B
- $V(x) = -u_1(x_1) + u_2(x_2,\dots,x_q) + \frac{1}{2}\sum_{j=q+1}^{d} \lambda_j x_j^2 + \cdots \qquad \lambda_j > 0$

$$\operatorname{cap}_A(B) = \varepsilon \frac{\displaystyle\int e^{-u_2(x_2,\dots,x_q)/\varepsilon}\,dx_2\dots dx_q}{\displaystyle\int e^{-u_1(x_1)/\varepsilon}\,dx_1} \prod_{j=q+1}^{d} \sqrt{\frac{2\pi\varepsilon}{\lambda_j}}\Bigl[1 + \mathcal{O}\bigl((\varepsilon|\log\varepsilon|)^{\alpha}\bigr)\Bigr]$$

with α related to growth of u_1 and u_2

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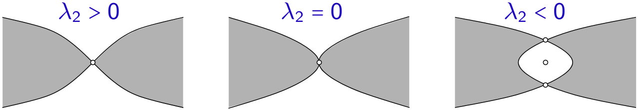
with α related to growth of u_1 and u_2

- ▷ Recall if $d\mu(x) = e^{-V(x)/\varepsilon}\,dx$ then
  $$\operatorname{cap}_A(B) = \int_{(A\cup B)^c} \|\nabla h_{A,B}(x)\|^2\,d\mu = \inf_{h\in\mathcal{H}_{A,B}} \int_{(A\cup B)^c} \|\nabla h(x)\|^2\,d\mu$$
- ▷ U.B.: $\operatorname{cap}_A(B) \leqslant \int_{(A\cup B)^c} \|\nabla h^*(x_1)\|^2\,d\mu$
  where $h^*(x_1)$ committor of 1D problem
- ▷ L.B.: $\operatorname{cap}_A(B) \geqslant \int_D (\partial_1 h_{A,B}(x))^2\,d\mu \geqslant \inf_{h|_{\partial D}=h_{A,B}} \int_D (\partial_1 h(x))^2\,d\mu$

Example – Transverse pitchfork bifurcation

$$V(x) = -\frac{1}{2}|\lambda_1|x_1^2 + \frac{1}{2}\lambda_2 x_2^2 + C_4 x_2^4 + \frac{1}{2}\sum_{j=3}^{d}\lambda_j x_j^2 + \cdots$$



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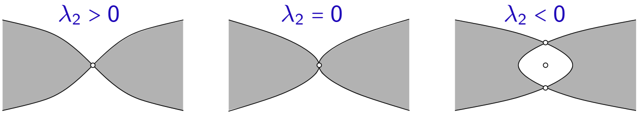


$$\mathbb{E}^x[\tau_B] = 2\pi\sqrt{\frac{(\lambda_2+\sqrt{2\varepsilon C_4})\lambda_3\dots\lambda_d}{|\lambda_1|\det(\nabla^2 V(x))}}\,\frac{e^{[V(0)-V(x)]/\varepsilon}}{\Psi_+(\lambda_2/\sqrt{2\varepsilon C_4})}\big[1+R(\varepsilon)\big]$$

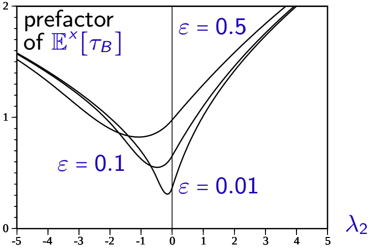
for $\lambda_2 > 0$ where

$\Psi_+(\alpha) = \sqrt{\frac{\alpha(1+\alpha)}{8\pi}}\, e^{\alpha^2/16} K_{1/4}\big(\frac{\alpha^2}{16}\big)$

$\lim_{\alpha\to+\infty}\Psi_+(\alpha) = 1$

$\lim_{\alpha\to 0}\Psi_+(\alpha) = \frac{\Gamma(1/4)}{2^{5/4}\pi^{1/2}} \simeq 0.860$

Similar expression for $\lambda_2 < 0$
with $\Psi_-(\alpha)$ involving $I_{\pm 1/4}$



Stochastic partial differential equations

$$\dot{u}_t(x) = \Delta u_t(x) + f(u_t(x)) \quad + \sqrt{2\varepsilon}\,\xi(t,x) \qquad (\Delta \equiv \partial_{xx}, f(u) = u - u^3)$$

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▷ $\dot{u}_t = \Delta u_t \qquad \Rightarrow \qquad u_t = e^{\Delta t} u_0$
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$$w_t(x) = \sum_k \int_0^t e^{-(k\pi/L)^2(t-s)}\, dW_s^{(k)} \cos\left(\frac{k\pi x}{L}\right) \in H^s \cap \mathcal{C}^\alpha \; \forall s, \alpha < \frac{1}{2}$$

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- $\dot{u}_t = \Delta u_t + \sqrt{2\varepsilon}\,\xi(t,x) + f(u_t)$

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$\Rightarrow$ Existence and a.s. uniqueness [Faris & Jona-Lasinio 1982]

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Fourier variables: $u_t(x) = \frac{1}{\sqrt{L}} \sum_{k=-\infty}^{\infty} z_k(t)\, \mathrm{e}^{\mathrm{i}\pi kx/L}$

$$\Rightarrow \qquad \mathrm{d}z_k = -\lambda_k z_k\,\mathrm{d}t - \frac{1}{L}\sum_{k_1+k_2+k_3=k} z_{k_1} z_{k_2} z_{k_3}\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t^{(k)}$$

Itō SDE, $\mathrm{d}W_t^{(k)}$: independent Wiener processes
$\lambda_k = -1 + (\pi k/L)^2$

Energy functional:

$$V[u] = \frac{1}{2}\sum_{k=-\infty}^{\infty} \lambda_k |z_k|^2 + \frac{1}{4L}\sum_{k_1+k_2+k_3+k_4=0} z_{k_1} z_{k_2} z_{k_3} z_{k_4}$$

$$\Rightarrow \qquad \mathrm{d}z_t = -\nabla V(z_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Eyring–Kramers law for 1D SPDEs: heuristics

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Initial condition: $u_{\rm in}$ near $u_- \equiv -1$ with eigenvalues ν_k

Target: $u_+ \equiv 1$, $\tau_+ = \inf\{t > 0\colon \|u_t - u_+\|_{L^\infty} < \rho\}$

Transition state: ($\beta = 1$ for Neumann b.c., $\beta = 2$ for periodic b.c.)

$$u_{\rm ts}(x) = \begin{cases} u_0(x) \equiv 0 & \text{if } L \leqslant \beta\pi \quad \text{with ev } \lambda_k = (\frac{\beta k\pi}{L})^2 - 1 \\ u_1(x) \ \beta\text{-kink stationary sol.} & \text{if } L > \beta\pi \quad \text{with ev } \lambda'_k \end{cases}$$

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[Faris & Jona-Lasinio 82]: large-deviation principle

$\Rightarrow$ Arrhenius law: $\mathbb{E}^{u_{\text{in}}}[\tau_+] \simeq e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon}$

[Maier & Stein 01]: formal computation; for Neumann b.c.

$$\Rightarrow \mathbb{E}^{u_{\text{in}}}[\tau_+] \simeq 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}}\, e^{(V[u_{\text{ts}}] - V[u_-])/\varepsilon}$$

- Rigorous proof?
- What happens when $L \to \beta\pi$ as then $\lambda_1 \to 0$?

Eyring–Kramers law for 1D SPDEs: main results

Theorem 1: Neumann b.c. [B & Gentz, Elec J Proba 2013]

- If $L < \pi - c$ with $c > 0$, then

$$\mathbb{E}^{u_{\rm in}}[\tau_+] = 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}}\, \mathrm{e}^{(V[u_{\rm ts}]-V[u_-])/\varepsilon} \Big[1 + \mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|^{3/2})\Big]$$

- If $L > \pi + c$, extra factor $\frac{1}{2}$, λ_k' instead of λ_k
- If $|L - \pi| \leqslant c$, similar expression involving Bessel functions

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- If $L > \pi + c$, extra factor $\frac{1}{2}$, λ'_k instead of λ_k
- If $|L - \pi| \leqslant c$, similar expression involving Bessel functions

Theorem 2: periodic b.c. [B & Gentz, Elec J Proba 2013]

- If $L < 2\pi - c$, same expression but double eigenvalues
- If $2\pi - c \leqslant L \leqslant 2\pi + c$, expressions involving error function
- If $L \geqslant 2\pi + c$, then

$$\mathbb{E}^{u_{\rm in}}[\tau_+] = \frac{2\pi}{\sqrt{|\lambda_0|\nu_0}} \frac{\sqrt{2\pi\varepsilon\lambda_1}}{\nu_1} \prod_{k=2}^{\infty} \frac{\sqrt{\lambda_k\lambda_{-k}}}{\nu_k} \frac{\mathrm{e}^{(V[u_{\rm ts}]-V[u_-])/\varepsilon}}{L\|u'_{\rm ts}\|_{L^2}} \big[1 + R(\varepsilon)\big]$$

$L\|u'_{\rm ts}\|_{L^2}$ = "length of the saddle"

Sketch of proof: Spectral Galerkin approximation

$u_t^{(d)}(x) = \frac{1}{\sqrt{L}} \sum_{k=-d}^{d} z_k(t) \, e^{i\pi kx/L} \quad \Rightarrow \quad dz_t = -\nabla V(z_t) \, dt + \sqrt{2\varepsilon} \, dW_t$

Theorem [Blömker & Jentzen 13]

For all $\gamma \in (0, \frac{1}{2})$ there exists an a.s. finite r.v. $Z : \Omega \to \mathbb{R}_+$ s.t. $\forall \omega \in \Omega$

$$\sup_{0 \leqslant t \leqslant T} \| u_t(\omega) - u_t^{(d)}(\omega) \|_{L^\infty} < Z(\omega) d^{-\gamma} \qquad \forall d \in \mathbb{N}$$

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Proposition (using potential theory)

$\exists \varepsilon_0 > 0 \colon \forall \varepsilon < \varepsilon_0\ \exists d_0(\varepsilon) < \infty \colon \forall d \geqslant d_0\ \exists \nu_d$ proba measure on $\partial\mathcal{B}_r(u_-)$

$$\int_{\partial\mathcal{B}_r(u_-)} \mathbb{E}^{v_0}[\tau_+^{(d)}]\nu_d(dv_0) = C(d,\varepsilon)\, e^{H(d)/\varepsilon}\big[1 + R(\varepsilon)\big]$$

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Proposition (using large deviations and lots of other stuff)

$H_0 := V[u_{\text{ts}}] - V[u_-]$. $\forall \eta > 0$ $\exists \varepsilon_0, T_1, H_1$: $\forall \varepsilon < \varepsilon_0$ $\exists d_0 < \infty$ s.t. $\forall d \geqslant d_0$

$$\sup_{v_0 \in \mathcal{B}_r(u_-)} \mathbb{E}^{v_0}[\tau_+^2] \leqslant T_1^2\, e^{2(H_0+\eta)/\varepsilon} \ , \ \sup_{d \geqslant d_0} \sup_{v_0 \in \mathcal{B}_r(u_-)} \mathbb{E}^{v_0}[(\tau_+^{(d)})^2] \leqslant T_1^2\, e^{2H_1/\varepsilon}$$

Main step of the proof

Set $T_{\mathrm{Kr}} = C(\infty, \varepsilon)\,\mathrm{e}^{H_0/\varepsilon}$

Let $B = \mathcal{B}_\rho(u_+)$ and define nested sets $B_- \subset B \subset B_+$ at L^∞-distance δ

$$\Omega_{K,d} = \left\{ \sup_{t\in[0,KT_{\mathrm{Kr}}]} \|v_t - v_t^{(d)}\|_{L^\infty} \leqslant \delta, \tau_{B_-}^{(d)} \leqslant KT_{\mathrm{Kr}} \right\}$$

$$\mathbb{P}(\Omega_{K,d}^c) \leqslant \mathbb{P}\{Z > \delta d^\gamma\} + \frac{\mathbb{E}^{v_0^{(d)}}\left[\tau_{B_-}^{(d)}\right]}{KT_{\mathrm{Kr}}} \quad \overset{\text{Cauchy–Schwarz}}{\Rightarrow} \quad \limsup_{d\to\infty} \mathbb{P}(\Omega_{K,d}^c) = \frac{M(\varepsilon)}{K}$$

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$\Rightarrow$

$$\mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)}] - \mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)} 1_{\{\Omega_{K,d}^c\}}] \leqslant \mathbb{E}^{v_0}[\tau_B] \leqslant \mathbb{E}^{v_0^{(d)}}[\tau_{B_-}^{(d)}] + \mathbb{E}^{v_0}[\tau_B 1_{\{\Omega_{K,d}^c\}}]$$

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$$\Rightarrow$$

$$\mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)}] - \mathbb{E}^{v_0^{(d)}}[\tau_{B_+}^{(d)} 1_{\{\Omega_{K,d}^c\}}] \leqslant \mathbb{E}^{v_0}[\tau_B] \leqslant \mathbb{E}^{v_0^{(d)}}[\tau_{B_-}^{(d)}] + \mathbb{E}^{v_0}[\tau_B 1_{\{\Omega_{K,d}^c\}}]$$

Integrate against ν_d and use Cauchy–Schwarz to bound error terms: $\mathbb{E}^{v_0}[\tau_B 1_{\{\Omega_{K,d}^c\}}] \leqslant \sqrt{\mathbb{E}^{v_0}[\tau_B^2]\mathbb{P}(\Omega_{K,d}^c)}$, take $d \to \infty$ and finally K large

Allen–Cahn in higher dimension

$$\partial_t u(t,x) = \Delta u(t,x) + u(t,x) - u(t,x)^3 + \sqrt{2\varepsilon}\xi(t,x) \qquad x \in \mathbb{T}^d$$

Theorem: [Da Prato & Debussche 2003]

$d = 2$. Let ξ^δ be a mollification on scale δ of white noise. Then

$$\partial_t u = \Delta u + \left[1 + 3\varepsilon C(\delta)\right] u - u^3 + \sqrt{2\varepsilon}\xi^\delta$$

with $C(\delta) \simeq \log(\delta^{-1})$ admits local solution converging as $\delta \to 0$
(Global version: [Mourrat & Weber 2015])

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Theorem: [Hairer 2014]

$d = 3$. Let ξ^δ be a mollification on scale δ of white noise. Then

$$\partial_t u = \Delta u + \big[1 + 3\varepsilon C_1(\delta) - 9\varepsilon^2 C_2(\delta)\big]u - u^3 + \sqrt{2\varepsilon}\xi^\delta$$

with $C_1(\delta) \simeq \delta^{-1}$, $C_2(\delta) \simeq \log(\delta^{-1})$ admits loc. solution conv. as $\delta \to 0$

Renormalisation for $d = 2$

Problem: Stoch. convolution $w_t(x) = \int_0^t e^{\Delta(t-s)} \xi(s,x) \, ds$ is a distribution

- δ-mollification should be equivalent to Galerkin approx. $|k| \leqslant N = \delta^{-1}$:

$$w_N(x,t) = \sum_{|k|\leqslant N} a_k(t) \frac{1}{L} e^{i\Omega k\cdot x} \qquad a_k = \int_0^t e^{-\mu_k(t-s)} \, dW_s^{(k)}$$

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- $\lim_{t\to\infty} \int_0^t e^{(\Delta-1)(t-s)} \xi_N(s,x)\,ds = \phi_N$ is a Gaussian free field, s.t.

$$L^2 C_N := L^2 \mathbb{E}\phi_N^2 = \mathbb{E}\|\phi_N\|_{L^2}^2 = \sum_{|k|\leqslant N} \frac{1}{2(\mu_k+1)} = \frac{\mathrm{Tr}(P_N[-\Delta+\mathbb{1}]^{-1})}{2} \simeq \log(N)$$

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- Wick powers

$$:\phi_N^2: = \phi_N^2 - C_N$$
$$:\phi_N^3: = \phi_N^3 - 3C_N\phi_N$$
$$:\phi_N^4: = \phi_N^4 - 6C_N\phi_N^2 + 3C_N^2$$

have zero mean and uniformly bounded variance (when integrated)

Nelson's estimate

Lemma For X random variable in n^{th} inhomogeneous Wiener chaos

$$\mathbb{E}[X^{2p}]^{\frac{1}{2p}} \leqslant C_n(2p-1)^{\frac{n}{2}}\mathbb{E}[X^2]^{\frac{1}{2}}$$

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Corollary

$$\mathbb{E}\Big[\exp\Big\{-\frac{\varepsilon}{4}\int_{\mathbb{T}^2} :\phi_N^4(x): \mathrm{d}x\Big\}\Big] \leqslant 1 + \mathcal{O}(\varepsilon)$$

- Integrand is bounded below by term of order $-C_N^2$
- Use Markov's ineq to bound tails of integral and integrate by parts

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- ▷ Use Markov's ineq to bound tails of integral and integrate by parts

Useful as $\mathrm{cap}_A(B) \leqslant \sqrt{\frac{|\lambda_0|\varepsilon}{2\pi}} \prod_{0<|k|\leqslant N} \sqrt{\frac{2\pi\varepsilon}{\lambda_k}}\mathbb{E}\Big[\exp\Big\{-\frac{\varepsilon}{4}\int_{\mathbb{T}^2} :u_N^4(x): \mathrm{d}x\Big\}\Big]$

Computation of the prefactor

- ▷ Consider for simplicity $L < \beta\pi \Rightarrow$ transition state in 0
- ▷ Galerkin-truncated renormalised potential

$$V_N = \frac{1}{2}\int_{\mathbb{T}^2}\left[\|\nabla u_N(x)\|^2 - u_N(x)^2\right]\mathrm{d}x + \frac{1}{4}\int_{\mathbb{T}^2} :u_N(x)^4: \mathrm{d}x$$

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$$\int_{B^c} h_{A,B}(z)\,\mathrm{e}^{-V_N(z)/\varepsilon}\,\mathrm{d}z = \frac{1}{2}\int \mathrm{e}^{-V_N(z)/\varepsilon}\,\mathrm{d}z = \frac{1}{2}\mathcal{Z}_N(\varepsilon)$$

- ▷ $\mathcal{Z}_N(\varepsilon) \simeq 2\prod_{|k|\leqslant N}\sqrt{\frac{2\pi\varepsilon}{\nu_k}}\,\mathrm{e}^{-V_N(L,0)/\varepsilon}$ where $-V_N(L,0) = \frac{1}{4}L^2 + \frac{3}{2}L^2 C_N\varepsilon$

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- Prefactor proportional to (since $\nu_k = \lambda_k + 3$)

$$\prod_{0<|k|\leqslant N} \frac{\lambda_k}{\lambda_k+3}\mathrm{e}^{3/\lambda_k} \qquad \text{converges since} \qquad \log\left[\frac{\lambda_k}{\lambda_k+3}\mathrm{e}^{3/\lambda_k}\right] = \mathcal{O}\left(\frac{1}{|k|^4}\right)$$

Main result in dimension 2

Theorem: [B, Di Gesù, Weber 2016]

For appropriate $A \ni u_-$, $B \ni u_+$, $\exists \mu_N$ probability measures on ∂A:

$$\limsup_{N\to\infty} \mathbb{E}^{\mu_N}\big[\tau_B\big] \leqslant \frac{2\pi}{|\lambda_0|}\sqrt{\prod_{k\in\mathbb{Z}^2} \frac{|\lambda_k|}{\nu_k}\, e^{\frac{\nu_k-\lambda_k}{|\lambda_k|}}}\, e^{(V[u_{\text{ts}}]-V[u_-])/\varepsilon}\big[1 + c_+\sqrt{\varepsilon}\,\big]$$

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(Inverse of) prefactor involves Carleman–Fredholm determinant:

$$\det_2(\mathrm{Id} + T) = \det(\mathrm{Id} + T)\mathrm{e}^{-\operatorname{Tr} T}$$

Defined whenever T is Hilbert–Schmidt, but not necessarily trace class

Applied here to $T = [(-\Delta + 2) - (-\Delta - 1)](|-\Delta - 1|)^{-1} = 3(|-\Delta - 1|)^{-1}$

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$d = 3$: no Nelson estimate

$\Rightarrow$ use perturbation theory to compute capacity and $\mathcal{Z}_N$?

References

For this talk: [1–5]; overview: [6]; symmetry group: [7,8]; non-reversible: [9]

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